

The extension of Fock's method of hydrogen atom treatment to one-dimensional case

Boris Ivetić*

Rudjer Bošković Institute,

Bijenička cesta 54, HR-10002 Zagreb, Croatia

and Dipartimento di Matematica e Informatica, Università di Cagliari,
viale Merello 92, 09123 Cagliari, Italy

Abstract

The quantum mechanical one-dimensional (1D) Coulomb-like potential $1/|x|$ is treated in this paper by direct Fourier transformation of the Schrödinger equation. To this purpose, a specific regularization technique is introduced, the solutions turning out to be independent of the regularization parameter. Projecting the momentum space from the real line on the circle, in an analogy with Fock's treatment of the 3D case, the equation is found to admit an $O(2)$ symmetry. This symmetry is responsible for the double degeneracy of energy levels. Employing the boundary condition of vanishing wave function at infinite momenta, the symmetry spontaneously breaks, removing the unwanted degeneracy.

1 Introduction

In 1935, Fock solved the problem of a hydrogen atom in momentum representation by projecting the three-dimensional momentum space on the surface of the three-dimensional sphere [1]. His original motivation was to find the group of transformations that explains the independence of the energy levels on the azimuthal quantum number. He identified this symmetry group with $O(4)$, the rotation group in the four-dimensional Euclidean space¹.

The method was then successfully generalized to the case of $D \geq 2$ dimensions by Alliluev [3] in 1958, and has since then been confirmed by other approaches [4, 5]. At the same time, the problem of the hydrogen atom in one dimension is plagued by the singular nature of the potential $1/|x|$ at the origin, that makes it difficult to treat by Fock's method. To the best of our knowledge, until today there was only one attempt of the extension of Fock's method to the case of 1D hydrogen atom²[11]. However, their findings, although in agreement with ours, were discarded on account of the inconsistency of their methodology, that was pointed out in [12]. It has since been the topic of controversy and disagreement between different authors

*bivetic@irb.hr

¹Some authors believe that the deep nature of this symmetry has yet to be understood [2]

²It is probably better to call it 1D "Coulomb-like potential", as the electrostatic potential of the point charge would look different in $d \neq 3$ dimensions. Here we only convey to the usual practice.

[6, 7, 8, 9, 10, 12, 13, 14, 15, 17]. Every once in a while, a new paper emerges pointing out the inconsistencies in the previous works and claiming that its approach finally solves this problem (a nice and thorough account of the historical development of this problematic can be found in [17]). Though at present there is still some controversy (as reported in [17]), there is a large agreement about how the solutions should look like. Therefore, we shall here avoid the unfortunate practice of claiming that we finally solve the problem and remove all the discrepancies. Rather, we adopt the more modest attitude to present the problem in its natural setting, by the extension of the beautiful method developed by Fock to the case of one dimension. Particular advantage of this approach is the explanation of appearance and also disappearance (spontaneous breakdown) of the double degeneracy between even and odd parity solutions.

We would also like to point out that the problem of the one-dimensional hydrogen atom is today no longer of purely academic interest. The number of physical systems that essentially exhibit 1D behaviour is growing (nanowires, trapped ions in laser created 1D potential, 1D systems in materials science, to name just a few), and it is not unlikely that interactions, impurities or irregularities of such systems could be described by an effective Coulomb-like potential.

The plan of the paper is as follows. In Section 2, we present the Fourier transform of the Schroedinger equation, using a specific regularization prescription to handle the singular $1/|x|$ potential. In section 3, we project the problem from the real line on the circle, using the parametrization of Fock. We conjecture the solutions to be spherical harmonics on a circle, in an analogy with higher dimensions, implying the existence of an $O(2)$ symmetry in the one-dimensional case. The proof is given by going back to the real line. The solutions turn out to be independent on the regularization parameter, allowing us to take it to its limit value zero, thus justifying our regularization method. Finally, using only the boundary condition of vanishing of the wave-function at infinite values of the momentum, we reject one of the solutions as unphysical, leaving the $O(2)$ symmetry spontaneously broken. Section 4 summarizes our findings and gives a short conclusion to the paper.

2 The Fourier transformed Schroedinger equation

The Schroedinger equation of the 1D hydrogen atom is

$$\frac{1}{2m'} \frac{d^2}{dx'^2} \psi(x') - \frac{e^2}{|x'|} \psi(x') = E' \psi(x'). \quad (1)$$

To Fourier transform this equation we would need the Fourier transform of $1/|x'|$, which does not exist. When written explicitly, it is

$$\frac{1}{|x'|} \rightarrow \frac{\sqrt{2}}{\pi} \int_0^\infty \frac{\cos(p'x')}{x'} dx',$$

with the above integral logarithmically divergent due to the singularity at the origin. It is this mathematical nuance that makes the extension of the Fock's treatment to the 1D case difficult. Noting that we actually need the Fourier transform of $\psi(x')/|x'|$ (which turns out to exist, see the coordinate space solutions in [17]), we proceed by employing the following regularization [18]

$$\frac{1}{|x'|} \rightarrow \frac{\sqrt{2}}{\pi} \int_{\epsilon}^{\infty} \frac{\cos(p'x')}{x'} dx' = -\frac{\sqrt{2}}{\pi} \left(\log |\epsilon p'| + \gamma + \sum_{k=1}^{\infty} \frac{(-(\epsilon p')^2)^k}{2k(2k)!} \right)$$

where ϵ is a small positive parameter (to be taken as zero upon finding the solutions) and γ is the Euler-Mascheroni constant. For all finite values of the momentum, the sum in the above expression vanishes once ϵ is taken to be zero. We can therefore safely neglect it. If we take the Fourier transform of the wave function to be

$$\psi(x') \rightarrow \phi(p'),$$

then

$$\frac{1}{|x'|} \psi(x') \rightarrow -\frac{\sqrt{2}}{\pi} \int_{-\infty}^{\infty} dp'' \log |\epsilon p'' - \epsilon p'| \phi(p'') - \frac{\sqrt{2}}{\pi} \gamma \int_{-\infty}^{\infty} dp'' \phi(p'')$$

To make our expressions simpler, we define a dimensionless momentum $p = \epsilon p'$. Scaling of momentum by a scale ϵ requires scaling of all other dimensionful quantities appearing in our problem, accordingly, by the same scale, i.e. $m = \epsilon m'$, $x = x'/\epsilon$, $E = \epsilon E'$. Now, the Fourier transformed version of equation (1) is

$$\frac{p^2}{2m} \phi(p) + \frac{\sqrt{2}e^2}{\pi} \int_{-\infty}^{\infty} dp' \log |p' - p| \phi(p') + \frac{\sqrt{2}}{\pi} \gamma \int_{-\infty}^{\infty} dp' \phi(p') = E \phi(p), \quad (2)$$

where the prime on p denotes the dummy variable of integration, not to be confused with the dimensionful momentum.

The last term on the LHS is just a constant. The solutions will be such that it will vanish (see appendix). From now on, we leave it out for simplicity. Defining a positive constant $p_0^2 = -2mE$, makes the equation (2)

$$(p^2 + p_0^2) \phi(p) = -2me^2 \frac{2}{\pi} \int_{-\infty}^{\infty} dp' \log |p' - p| \phi(p') \quad (3)$$

3 Fock's method in 1D

Following the idea of Fock, we project the momentum space from \mathbf{R}^1 to \mathbf{S}^1 . We define an angle α by

$$\sin \alpha = \frac{2p_0 p}{p_0^2 + p^2} \quad \cos \alpha = \frac{p_0^2 - p^2}{p_0^2 + p^2}, \quad (4)$$

with an inverse relation

$$p = p_0 \tan \frac{\alpha}{2},$$

and with the range of α from $-\pi$ ($p \rightarrow -\infty$) to π ($p \rightarrow \infty$). Note that angle α is defined in a scale-invariant way.

The infinitesimal elements are related by

$$dp = \frac{p_0^2 + p^2}{2p_0^2} d\alpha.$$

Defining a new wave function in terms of the variable α as

$$\phi(\alpha) = \frac{p_0^2 + p^2}{2p_0^2} \phi(p), \quad (5)$$

where the factor is chosen so that the normalization condition³

$$\frac{1}{2\pi} \int d\alpha |\phi(\alpha)|^2 = \frac{1}{2\pi} \int dp' \frac{p'^2 + p_0^2}{2p_0^2} |\phi(p')|^2 = \int dx' |\psi(x')|^2$$

is satisfied, turns equation (3) into

$$\phi(\alpha) = -\frac{2me^2}{p_0^2\pi} \int_{-\pi}^{\pi} d\alpha' \phi(\alpha') \log \left| p_0 \left(\tan \frac{\alpha'}{2} - \tan \frac{\alpha}{2} \right) \right|. \quad (6)$$

In complete analogy with higher dimensional cases, we guess the solutions of this equation to be spherical harmonics on the circle. These are just the sines and cosines:

$$\phi^-(\alpha) = c_1 \sin(n\alpha), \quad \phi^+(\alpha) = c_1 \cos(n\alpha), \quad (7)$$

c_1 being an arbitrary constant. That these indeed solve equation (6) is most readily seen by going back to the real line. It is easy to show using mathematical induction that

$$\begin{aligned} \sin(n\alpha) &= \frac{1}{2i} \left[\left(\frac{p_0 - ip}{p_0 + ip} \right)^n - \left(\frac{p_0 + ip}{p_0 - ip} \right)^n \right] \\ \cos(n\alpha) &= \frac{1}{2i} \left[\left(\frac{p_0 - ip}{p_0 + ip} \right)^n + \left(\frac{p_0 + ip}{p_0 - ip} \right)^n \right]. \end{aligned}$$

This would give two linearly independent solutions of the momentum-space (the real line) integral equation

$$\phi_n^\pm(p, p_0) = c \frac{p_0^2}{p^2 + p_0^2} \left[\left(\frac{p_0 - ip}{p_0 + ip} \right)^n \pm \left(\frac{p_0 + ip}{p_0 - ip} \right)^n \right], \quad (8)$$

with c an arbitrary (normalization) constant. It can be shown that these really are the solutions of eq. (3) by a direct substitution. The evaluation of the integral on the RHS of (3) is shortly reported in the appendix, with explicit expressions for the values of various residua given. The eigenvalues are given by $p_0^2 = 2m^2 e^4 / n^2$, where n is an integer different from zero.

One sees from the shape of the solutions that they are in fact scale-invariant:

$$\phi_n^\pm(p, p_0) = \phi_n^\pm(\epsilon p', \epsilon p'_0) = \phi_n^\pm(p', p'_0)$$

and also

$$E = -\frac{me^4}{n^2} \rightarrow E' = -\frac{m'e^4}{n^2},$$

so that we may safely let ϵ to its limit value zero.

The solutions are the symmetric and antisymmetric combinations of the solutions firstly found by Nunez-Yepe et al [10]. The antisymmetric combination is the only one allowed by the boundary conditions, as is correctly reported in [17].

³The primed variables are here the physical ones.

3.1 Boundary conditions

The requirement that the wavefunction $\phi(\alpha)$ should vanish as the momenta go to infinity ($\alpha \rightarrow \pm\pi$), leaves us with sines as the only physically allowed solution. This confirms the solution given in the most recent paper on the problem, by Palma and Raff [17]. We find that removing the degeneracy in our approach is more elegant than in the other approaches found in the literature. It is given without resorting to "fixing" the potential to make it physical [16], speculation about the penetrability of $x = 0$ barrier [10], requirement of square integrability of wave functions [17], or more mathematically sophisticated methods such as functional-analytic approach [13], or self-adjoint extension used in other papers [14, 15]. In all of the papers we came across, the focus was put to the more demanding coordinate representation boundary condition at $x = 0$, which is in our approach entirely avoided, fully exploiting the duality nature of coordinate and momentum representations. As the parity is preserved in a Fourier transform, the parity analysis in momentum space is also completely equivalent to the one in coordinate space⁴.

It is also readily seen that equation (6) admits an $O(2)$ symmetry. This "secret" symmetry is the one that is responsible for the double degeneracy of the energy levels (for dimensions $D \geq 2$, see [3]), that was the biggest problem in 1D hydrogen atom treatment. By choosing the appropriate boundary conditions at infinite momenta, this symmetry is spontaneously broken, leaving only odd parity solutions as the physically acceptable ones.

4 Conclusion

We have found solutions to the 1D hydrogen atom problem in momentum representation, by means of a Fourier transform of the Schroedinger equation, using the regularization at the origin. The solutions agree with the ones existing in the literature [11, 17]. The recognition of the $O(2)$ symmetry admitted by the equation in momentum space as the one responsible for the double degeneracy of the energy levels was done by pushing the analogy to the familiar $SO(D + 1)$ symmetry in D dimension, with $D \geq 2$ [3]. It thus confirms the finding of [11], by an alternative approach, avoiding the critique of their method in [12].

Finally, we were not able to show that the solutions (7) solve eq. (6) directly integrating over the variable α' . Confirming the solutions indirectly, we suspect that (6)+(7) might present novel (we weren't able to find it tabulated) integral relations for the Chebyshev polynomials:

$$T_n(x) = \frac{-n^2}{\pi\epsilon} \int_{-1}^1 dx' T_n(x') \log \left| \frac{\sqrt{2}\epsilon}{n} \left(\frac{\sqrt{1-x'^2}}{1+x'} - \frac{\sqrt{1-x^2}}{1+x} \right) \right|$$

$$\sqrt{1-x^2} U_{n-1}(x) = \frac{-n^2}{\pi\epsilon} \int_{-1}^1 dx' \sqrt{1-x'^2} U_{n-1}(x') \log \left| \frac{\sqrt{2}\epsilon}{n} \left(\frac{\sqrt{1-x'^2}}{1+x'} - \frac{\sqrt{1-x^2}}{1+x} \right) \right|,$$

which hold for every ϵ .

⁴It is unclear to us why the boundary conditions weren't considered in [11]. Our guess is that the authors were only interested in explaining the mechanism behind the degeneracy, and not its removal.

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Appendix

Defining the variable $z = p' - p$, the integral on the RHS of equation (3) is

$$I \equiv \int_{-\infty}^{\infty} dp' \phi_n(p') \log |p - p'| = \int_{-\infty}^0 dz (\phi_n(z + p) + \phi_n(-z + p)) \log(-z). \quad (9)$$

Our advocated solutions (8), neglecting the constant in front, can be put in the form

$$\phi_n^{\pm}(p') = (-1)^n p_0^2 \left[\frac{(p' + ip_0)^{n-1}}{(p' - ip_0)^{n+1}} \pm \frac{(p' - ip_0)^{n-1}}{(p' + ip_0)^{n+1}} \right].$$

From this form it is visible that the requirement for the vanishing of constant contribution in (3) is satisfied by our solutions. The integrand has no residue, and closing the contour in upper/lower half-plane with an infinite radius semi-circle gives

$$\int_{-\infty}^{\infty} dp \phi_n^{\pm}(p) = 0.$$

With the introduction of a constant $A \equiv -p + ip_0$ we have

$$\begin{aligned} \phi_n^{\pm}(z + p) + \phi_n^{\pm}(-z + p) &= (-1)^n p_0^2 \left[\frac{(z - A^*)^{n-1}}{(z - A)^{n+1}} \pm \frac{(z - A)^{n-1}}{(z - A^*)^{n+1}} + \frac{(z + A^*)^{n-1}}{(z + A)^{n+1}} \pm \frac{(z + A)^{n-1}}{(z + A^*)^{n+1}} \right] \\ &\equiv (-1)^n p_0^2 (f_1(z) \pm f_2(z) + f_3(z) \pm f_4(z)) \\ &\equiv (-1)^n p_0^2 F^{\pm}(z). \end{aligned}$$

To evaluate I^{\pm} , we shall use the standard trick to evaluate

$$\int_{\Gamma} dz F^{\pm}(z) \log^2(-z)$$

over the familiar "keyhole" or "Pacman" contour encircling the negative real axes just above and just below the logarithm cut. This gives

$$I^{\pm} = (-1)^n p_0^2 \frac{1}{2} \sum \text{Res} (F^{\pm}(z) \log^2(-z)).$$

The difficult part is evaluating the residue of the $(n - 1)$ -th order poles. This is best done using a power expansion of the integrand function, where care is needed in expansion of the logarithms. Since in complex plane

$$\log(z_1 z_2) = \log(z_1) + \log(z_2) + 2i\pi N,$$

where

$$N = \begin{cases} -1, & \text{if } \text{Arg} z_1 + \text{Arg} z_2 > \pi \\ 0, & \text{if } -\pi < \text{Arg} z_1 + \text{Arg} z_2 \leq \pi \\ 1, & \text{if } \text{Arg} z_1 + \text{Arg} z_2 \leq -\pi, \end{cases}$$

different signs of momentum p have to be treated separately (we take $p_0 > 0$). The values of the residua for negative values of momenta are

$$\begin{aligned}
\text{Res}(f_1, A) &= -2(2ip_0)^{n-1} \log(-A) \sum_{k=0}^{n-1} \binom{n-1}{k} \frac{(-1)^{n-k}}{n-k} \frac{1}{(2ip_0)^k A^{n-k}} \\
&\quad + (2ip_0)^{n-1} \sum_{k=0}^{n-1} \binom{n-1}{k} \frac{(-1)^{n-k}}{(2ip_0)^k A^{n-k}} \sum_{l=1}^{n-k-1} \frac{1}{l(n-k-l)} \\
\text{Res}(f_2, A*) &= -2(-2ip_0)^{n-1} \log(-A*) \sum_{k=0}^{n-1} \binom{n-1}{k} \frac{(-1)^{n-k}}{n-k} \frac{1}{(-2ip_0)^k (A*)^{n-k}} \\
&\quad + (-2ip_0)^{n-1} \sum_{k=0}^{n-1} \binom{n-1}{k} \frac{(-1)^{n-k}}{(-2ip_0)^k (A*)^{n-k}} \sum_{l=1}^{n-k-1} \frac{1}{l(n-k-l)} \\
\text{Res}(f_3, -A) &= -2(-2ip_0)^{n-1} \log(A) \sum_{k=0}^{n-1} \binom{n-1}{k} \frac{1}{n-k} \frac{1}{(-2ip_0)^k A^{n-k}} \\
&\quad + (-2ip_0)^{n-1} \sum_{k=0}^{n-1} \binom{n-1}{k} \frac{1}{(-2ip_0)^k A^{n-k}} \sum_{l=1}^{n-k-1} \frac{1}{l(n-k-l)} \\
\text{Res}(f_4, -A*) &= -2(2ip_0)^{n-1} \log(A*) \sum_{k=0}^{n-1} \binom{n-1}{k} \frac{1}{n-k} \frac{1}{(2ip_0)^k (A*)^{n-k}} \\
&\quad + (2ip_0)^{n-1} \sum_{k=0}^{n-1} \binom{n-1}{k} \frac{1}{(2ip_0)^k (A*)^{n-k}} \sum_{l=1}^{n-k-1} \frac{1}{l(n-k-l)}
\end{aligned}$$

with similar expressions in case $p > 0$. This gives (for both positive and negative momenta)

$$\sum \text{Res} (F^\pm(z) \log^2(-z)) = (-1)^{n+1} \frac{\pi}{np_0} \left[\left(\frac{p_0 - ip}{p_0 + ip} \right)^n \pm \left(\frac{p_0 + ip}{p_0 - ip} \right)^n \right],$$

which is precisely what is needed to satisfy (3).

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